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Poisson's Ratio for Cubic Crystals

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POISSON'S RATIO FOR CUBIC CRYSTALS

Abstract

General expressions for Poisson's ratio are derived for cubic crystals; simplified forms are given for cases involving symmetry directions.

Introduction

Poisson's ratio, ν, is defined for isotropic media as the quotient of lateral contraction to longitudinal extension arising from application of a simple tensile stress; in most materials, this dimensionless number is positive. In crystals, ν takes on different values, depending on the directions of stress and strain chosen. The ratio finds application in a variety of areas of applied elasticity and solid mechanics, for example, as indication of the mechanical coupling between various vibrational modes of motion.

The maximum value of $\nu = +1/2$ is obtained in the incompressible medium limit, where volume is preserved; for ordinary materials, values of $+1/4$ to $+1/3$ are typical, but in crystals ν may vanish, or take on negative values. Analytical formulas for Poisson's ratio are expressed in terms of elastic constants. For the case of crystals of general anisotropy, these expressions are quite unwieldy, but for cubic crystals the symmetry elements reduce the complexity considerably.

Crystals of cubic symmetry include many of the binary semiconductor systems with the piezoelectric zincblende structure, such as GaAs and related alloys. These are extremely important for high technology applications such as cellular radio and microwave collision avoidance radar. All cubic classes have the same elastic matrix scheme, so for our purposes it is not necessary to distinguish between the cubic point groups. The cubic elastic matrix scheme is identical in form to that of isotropic substances; the difference is that for isotropic materials the shear coefficient (s_{44} or c_{44}) is related to the two other independent coefficients, whereas in cubic crystals it is a third independent quantity.

Expressions Relating Cubic Stiffnesses and Compliances

Relations for Poisson's ratio are most simply expressed in terms of the elastic compliances $[s_{\lambda\mu}]$. It is often the case, however, that the most accurate determinations of the elastic constants (resonator and transit-time methods) yield values for the stiffnesses $[c_{\lambda\mu}]$ directly; the conversion relations are given below. For the cubic system, the elastic stiffness and compliance matrices have identical form. Referred to the [100], [010], and [001] directions, the matrices are:

$$\begin{matrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{matrix} \qquad \begin{matrix} s_{11} & s_{12} & s_{12} & 0 & 0 & 0 \\ s_{12} & s_{11} & s_{12} & 0 & 0 & 0 \\ s_{12} & s_{12} & s_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{44} \end{matrix}$$

Stiffness and compliance are matrix reciprocals; the three independent components of each are related by:

$$c_{11} = (s_{11} + s_{12}) / [(s_{11} - s_{12})(s_{11} + 2s_{12})]$$

$$c_{12} = (- s_{12}) / [(s_{11} - s_{12})(s_{11} + 2s_{12})]$$

$$c_{44} = 1 / s_{44}$$

These are inverted simply by an interchange of symbols $c_{\lambda\mu}$ and $s_{\lambda\mu}$. For the case of isotropy, one has the further relations $s_{44} = 2(s_{11} - s_{12})$ and $c_{44} = (c_{11} - c_{12})/2$. For cubic crystals, anisotropy factors $s = (s_{11} - s_{12} - s_{44}/2)$ and $c = (c_{11} - c_{12} - 2c_{44})$ are defined, in terms of which the departure from isotropy may be quantized. The Poisson's ratios are simply expressed in terms of s_{11}, s_{12}, and s.

Definition of Poisson's Ratio for Crystals

Poisson's ratio for crystals is defined in general as $\nu_{ji} = s_{ij}' / s_{jj}'$, where x_j is the direction of the longitudinal extension, x_i is the direction of the accompanying lateral contraction, and the s_{ij}' and s_{jj}' are the appropriate elastic compliances referred to this right-handed axial set. It suffices to take x_1 as the direction of the longitudinal extension; then two Poisson's ratios are defined by the orientations of the lateral axes x_2 and x_3: $\nu_{21} = s_{12}' / s_{11}'$ and $\nu_{31} = s_{13}' / s_{11}'$. Application of the definition requires

specification of the orientation of the x_k coordinate set with respect to the crystallographic directions, and transformation of the compliances accordingly.

Relations for Rotated Cubic Compliances - General

The unprimed compliances s_{11} , s_{44} , and s_{12} are referred to a set of right-handed cubic crystallographic axes aligned with the [100], [010], and [001] directions. Direction cosines a_{mn} relate the transformation from these axes to the set specifying the directions of the longitudinal extension (x_1), and the lateral contractions (x_2 and x_3). General expressions for the transformed compliances that enter the formulas for ν_{21} and ν_{31} are:

$$s_{11}' = s_{11} [a_{11}^4 + a_{12}^4 + a_{13}^4] + (s_{44} + 2 s_{12}) [a_{11}^2 a_{12}^2 + a_{12}^2 a_{13}^2 + a_{13}^2 a_{11}^2]$$

$$\begin{aligned} s_{12}' = {} & s_{11} [a_{11}^2 a_{21}^2 + a_{12}^2 a_{22}^2 + a_{13}^2 a_{23}^2] + \\ & s_{44} [a_{12} a_{13} a_{22} a_{23} + a_{13} a_{11} a_{23} a_{21} + a_{11} a_{12} a_{21} a_{22}] + \\ & s_{12} [a_{11}^2 a_{22}^2 + a_{12}^2 a_{21}^2 + a_{11}^2 a_{23}^2 + a_{13}^2 a_{21}^2 + a_{12}^2 a_{23}^2 + a_{13}^2 a_{22}^2] \end{aligned}$$

$$\begin{aligned} s_{13}' = {} & s_{11} [a_{11}^2 a_{31}^2 + a_{12}^2 a_{32}^2 + a_{13}^2 a_{33}^2] + \\ & s_{44} [a_{12} a_{13} a_{32} a_{33} + a_{13} a_{11} a_{33} a_{31} + a_{11} a_{12} a_{31} a_{32}] + \\ & s_{12} [a_{11}^2 a_{32}^2 + a_{12}^2 a_{31}^2 + a_{11}^2 a_{33}^2 + a_{13}^2 a_{31}^2 + a_{12}^2 a_{33}^2 + a_{13}^2 a_{32}^2] \end{aligned}$$

Single-Axis Rotations

The general rotation relations given above for s_{11}' , s_{12}' , and s_{13}' simplify considerably for single-axis rotations, and use of the anisotropy factor $s = (s_{11} - s_{12} - s_{44}/2)$. Longitudinal extension is along the x_1 axis, and abbreviations $c(\varphi)$ and $s(\varphi)$ stand for $\cos(\varphi)$ and $\sin(\varphi)$, etc.:

(A) Rotation about x_1: $s_{11}' = s_{11}$; $s_{12}' = s_{13}' = s_{12}$; $\nu_{21} = \nu_{31} = s_{12} / s_{11}$

(B) Rotation about x_2: $s_{11}' = s_{11} - 2 s [c^2(\psi) s^2(\psi)]$; $s_{12}' = s_{12}$

$s_{13}' = s_{12} + 2 s [c^2(\psi) s^2(\psi)]$; $\nu_{21} = s_{12} / s_{11}'$; $\nu_{31} = s_{13}' / s_{11}'$

(C) Rotation about x_3: $s_{11}' = s_{11} - 2 s [c^2(\varphi) s^2(\varphi)]$

$s_{12}' = s_{12} + 2 s [c^2(\varphi) s^2(\varphi)]$; $s_{13}' = s_{12}$; $\nu_{21} = s_{12}' / s_{11}'$; $\nu_{31} = s_{12} / s_{11}'$

Transformation Matrix for General Rotations

In order to derive the Poisson's ratio for the most general case, we consider the transformation matrix for a combination of three coordinate rotations: a first rotation about x_3 by angle φ, a second rotation about the new x_1 by angle θ, and a third rotation about the resulting x_2 by angle ψ. When these angles are set to zero, the x_1, x_2, x_3 axes coincide respectively with the [100], [010], and [001] crystallographic directions. For nonzero angles, the direction cosines a_{mn} are as follows:

$$
\begin{matrix}
[c(\varphi)c(\psi) - s(\varphi)s(\theta)s(\psi)] & [s(\varphi)c(\psi) + c(\varphi)s(\theta)s(\psi)] & [-c(\theta)s(\psi)] \\
[-s(\varphi)c(\theta)] & [c(\varphi)c(\theta)] & [\ s(\theta)\ ] \\
[c(\varphi)s(\psi) + s(\varphi)s(\theta)c(\psi)] & [s(\varphi)s(\psi) - c(\varphi)s(\theta)c(\psi)] & [\ c(\theta)c(\psi)]
\end{matrix}
$$

Substitution of these a_{mn} into the expressions for s_{11}' , s_{12}' , and s_{13}' , and thence into the formulas $\nu_{21} = s_{12}' / s_{11}'$ and $\nu_{31} = s_{13}' / s_{11}'$ formally solves the problem for specified values of φ, θ, and ψ.

Poisson's Ratios for Specific Orientations

1) Longitudinal extension along [100]: $\varphi = \psi = 0$; θ arbitrary. This is the same as case (A) above. $\nu_{21} = \nu_{31} = s_{12} / s_{11}$, independent of angle θ.

2) Longitudinal extension along an axis normal to [001]: $\psi = 0$; φ and θ arbitrary. Direction cosines are:

$$
\begin{matrix}
[c(\varphi)] & [s(\varphi)] & [0] \\
[-s(\varphi)c(\theta)] & [c(\varphi)c(\theta)] & [s(\theta)] \\
[s(\varphi)s(\theta)] & [-c(\varphi)s(\theta)] & [c(\theta)]
\end{matrix}
$$

Rotated compliances are:

$$s_{11}' = s_{11} - 2\,s\,[c^2(\varphi)\,s^2(\varphi)]$$

$$s_{12}' = s_{12} + 2\,s\,[c^2(\varphi)\,s^2(\varphi)\,c^2(\theta)]$$

$$s_{13}' = s_{12} + 2\,s\,[c^2(\varphi)\,s^2(\varphi)\,s^2(\theta)]$$

$$\nu_{21} = s_{12}' / s_{11}' ;\ \nu_{31} = s_{13}' / s_{11}'$$

2a) When both θ and $\psi = 0$, but φ is arbitrary, this reduces to case (C) above:

$$s_{11}' = s_{11} - 2\, s\, [c^2(\varphi)\, s^2(\varphi)]$$

$$s_{12}' = s_{12} + 2\, s\, [c^2(\varphi)\, s^2(\varphi)]$$

$$s_{13}' = s_{12}\ ;\ \nu_{21} = s_{12}' / s_{11}'\ ;\ \nu_{31} = s_{12} / s_{11}'$$

2b) When $\varphi = \pi/4$, θ is arbitrary, and $\psi = 0$, the x_1 axis (direction of longitudinal extension) coincides with the [110] direction; the rotated compliances become:

$$s_{11}' = s_{11} - s\,(1/2)\ ;\ s_{12}' = s_{12} + s\,(1/2)[c^2(\theta)]\ ;\ s_{13}' = s_{12} + s\,(1/2)[s^2(\theta)]$$

$$\nu_{21} = s_{12}' / s_{11}' = (2\, s_{12} + s\, [c^2(\theta)]) / (2\, s_{11} - s)$$

$$\nu_{31} = s_{13}' / s_{11}' = (2\, s_{12} + s\, [s^2(\theta)]) / (2\, s_{11} - s)$$

2c) When $\varphi = \pi/4$, $\theta = 0$, and $\psi = 0$, the x_1 axis (direction of longitudinal extension) coincides with the [110] direction, and the x_2 and x_3 axes coincide respectively with the [-110] and [001] directions. The rotated compliances then become:

$$s_{11}' = s_{11} - s\,(1/2)\ ;\ s_{12}' = s_{12} + s\,(1/2)\ ;\ s_{13}' = s_{12}$$

The Poisson's ratios are thus:

$$\nu_{21} = s_{12}' / s_{11}' = (2\, s_{12} + s) / (2\, s_{11} - s) \quad \text{and}$$

$$\nu_{31} = s_{13}' / s_{11}' = (2\, s_{12}) / (2\, s_{11} - s)$$

When $\theta = \pi/2$ instead of 0, ν_{21} and ν_{31} are simply interchanged.

3) Longitudinal extension in the plane containing [110] and [111]:
$\varphi = \pi/4$, $\theta = 0$, ψ arbitrary. The x_2 axis coincides with the [-110] direction. Direction cosines are:

$c(\psi)/\sqrt{2}$	$c(\psi)/\sqrt{2}$	$- s(\psi)$
$- 1/\sqrt{2}$	$1/\sqrt{2}$	0
$s(\psi)/\sqrt{2}$	$s(\psi)/\sqrt{2}$	$c(\psi)$

Rotated compliances are:

$$s_{11}' = s_{11} - 2\, s\, [c^2(\psi)]\, [\, 1 - (3/4)c^2(\psi)]$$

$$s_{12}' = s_{12} + (1/2)\, s\, [c^2(\psi)]$$

$$s_{13}' = s_{12} + (3/2)\, s\, [c^2(\psi)\, s^2(\psi)]$$

The Poisson's ratios are: $\nu_{21} = s_{12}' / s_{11}'$; $\nu_{31} = s_{13}' / s_{11}'$. When $\psi = 0$, this reduces to case 2c) above; when $\psi = \pi/2$, it is equivalent to case (A) with extension along [001].

4) Longitudinal extension along [-11-1]: $\varphi = \pi/4$, $\theta = 0$, and ψ = arc sin $(1/\sqrt{3})$. The x_2 and x_3 axes coincide, respectively, with the [-110] and [112] directions. Direction cosines a_{mn} are:

$1/\sqrt{3}$	$1/\sqrt{3}$	$- 1/\sqrt{3}$
$- 1/\sqrt{2}$	$1/\sqrt{2}$	0
$1/\sqrt{6}$	$1/\sqrt{6}$	$\sqrt{(2/3)}$

Rotated compliances are:

$$s_{11}' = s_{11} - (2/3)\, s$$

$$s_{12}' = s_{13}' = s_{12} + (1/3)\, s$$

The Poisson's ratios are: $\nu_{21} = \nu_{31} = s_{12}' / s_{11}' = (3\, s_{12} + s) / (3\, s_{11} - 2\, s)$

5) Longitudinal extension along [-11-1]: $\varphi = \pi/4$ and ψ = arc sin $(1/\sqrt{3})$. Provision is made for rotating the lateral axes by adding a third rotation, about the resulting x_1 (i.e., about [-11-1]), by angle θ, subsequent to the φ and ψ rotations.

Direction cosines a_{mn} are now:

$1/\sqrt{3}$	$1/\sqrt{3}$	$- 1/\sqrt{3}$
$1/\sqrt{2}\, [- c(\theta) + s(\theta)/\sqrt{3}]$	$1/\sqrt{2}\, [\, c(\theta) + s(\theta)/\sqrt{3}]$	$\sqrt{(2/3)}\, s(\theta)$
$1/\sqrt{2}\, [\, s(\theta) + c(\theta)/\sqrt{3}]$	$1/\sqrt{2}\, [\, - s(\theta) + c(\theta)/\sqrt{3}]$	$\sqrt{(2/3)}\, c\theta)$

Rotated compliances computed from these direction cosines turn out to be independent of angle θ, and are identical to those of case 4) above:

$$s_{11}' = s_{11} - (2/3)\, s$$

$$s_{12}' = s_{13}' = s_{12} + (1/3)\, s$$

The Poisson's ratios are: $\nu_{21} = \nu_{31} = s_{12}' / s_{11}' = (3\, s_{12} + s) / (3\, s_{11} - 2\, s)$

Conclusions

Poisson's ratio, with respect to rotated coordinate axes for cubic materials, has been obtained. Three cases are of particular interest:

- For longitudinal extension along [100] (along the cube axis), $\nu_{21} = \nu_{31} = s_{12} / s_{11}$, independent of lateral directions. Case (A).

- For longitudinal extension along [110] (along the face diagonal; normal to the dodecahedral planes (110)), with $s = (s_{11} - s_{12} - s_{44}/2)$,

$$\nu_{21} = (2\, s_{12} + s\, [c^2\,(\theta)]) / (2\, s_{11} - s)$$

$$\nu_{31} = (2\, s_{12} + s\, [s^2\,(\theta)]) / (2\, s_{11} - s)$$

When $\theta = 0$, the x_2 and x_3 axes coincide, respectively, with the [-110] and [001] directions. Case 2c). Poisson's ratios are:

$$\nu_{21} = (2\, s_{12} + s) / (2\, s_{11} - s)$$

$$\nu_{31} = (2\, s_{12}) / (2\, s_{11} - s)$$

- For longitudinal extension along [111] (along the body diagonal; normal to the octahedral planes (111)). Case 5). Poisson's ratios are independent of the lateral directions:

$$\nu_{21} = \nu_{31} = [3\, s_{12} + s\,] / [3\, s_{11} - 2\, s]$$

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